

Fermionic TAP-equations

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Abstract. We derive the TAP equations for the fermionic Ising spin glass. It is found that, just as in the non-fermionic model, the conditions for stability and for validity of the free energy are equivalent. We determine the breakdown of the paramagnetic phase. Numeric solutions of the fermionic TAP-equations at $T = 0$ allowed to localize a first order transition between the spin glass phase and the paramagnetic phase at $\mu \approx 0.8$. We computed at zero temperature the filling factor $\nu(\mu)$ and the distribution of internal fields. The saddle-point equations resulting from the calculation of the number of solutions to the TAP-equations were found to be much more complicated as in the non-fermionic case.

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Introduction

Thouless, Anderson and Palmer derived local mean-field equations for the random Ising model [18]. We generalize these TAP-equations to the four-state fermionic spin glass including a chemical potential μ . \tilde{n} is the number operator, J_{ij} are gaussian distributed random interactions with variance J^2/N :

$$\mathcal{H} = -\frac{1}{2} \sum_{ij} J_{ij} \sigma_i \sigma_j - \mu \sum_i \tilde{n}_i - \sum_i h_i^{ext} \sigma_i.$$

It is believed [2, 15], that the complete set of solutions to the TAP-equations is equivalent to the fully replica symmetry broken solution in the quantum-field theory [6, 7, 8, 9], so far only known for half filling. We were able to solve the fermionic TAP-equations numerically on the $T = 0$ axis and to determine the first order transition at $\mu_c \approx 0.8$ where the paramagnetic- and spin glass free energies become equal. The dependence of the filling factor on the chemical potential and the distribution of internal fields are given below.

1. Fermionic TAP-equations

The free energy corresponding to the non-fermionic TAP-equations is:

$$\begin{aligned} \mathcal{F} = & - \sum_i h_i^{ext} m_i - \frac{1}{2} \sum_{ij} J_{ij} m_i m_j - \frac{\beta}{4} \sum_{ij} J_{ij}^2 (1 - m_i^2)(1 - m_j^2) \\ & + \frac{1}{\beta} \sum_i \left\{ (1 + m_i) \ln\left(\frac{1 + m_i}{2}\right) + (1 - m_i) \ln\left(\frac{1 - m_i}{2}\right) \right\} \end{aligned} \quad (1)$$

In order to calculate the corresponding expression for the generalized fermionic model, we extended the linked cluster diagrammatic theory by Horwitz and Callen [3]. For the sake of simplicity this rigorous and lengthy derivation is replaced by shorter and more intuitive arguments.

The terms involving logarithms in equation (1) correspond to the entropy of an ensemble of spins in the non-fermionic two state model with relative occupations $n_{i\uparrow}$ and $n_{i\downarrow}$, using $m_i = n_{i\uparrow} - n_{i\downarrow}$. Now we replace these terms with the entropy of the ensemble in the extended fermionic four state model. The relative occupations are denoted by $n_{i\uparrow}$, $n_{i\downarrow}$, n_{i0} and $n_{i\uparrow\downarrow}$, setting $m_i = n_{i\uparrow} - n_{i\downarrow}$, $n_i = n_{i\uparrow} + n_{i\downarrow} + 2n_{i\uparrow\downarrow}$ and $\tilde{q}_i = n_{i\uparrow} + n_{i\downarrow}$. Then we account for the non-trivial occupation number of the magnetic states by replacing $1 - m_i^2$ in the Onsager reaction field by $\tilde{q}_i - m_i^2$. After a final Legendre transformation the fermionic free energy reads

$$\begin{aligned}
\mathcal{F} = & -\frac{1}{2} \sum_{ij} J_{ij} m_i m_j - \frac{\beta}{4} \sum_{ij} J_{ij} (\tilde{q}_i - m_i^2)(\tilde{q}_j - m_j^2) - \sum_i \mu(1 + (1 - \tilde{q}_i) \mathbb{T}) + \frac{N}{\beta} \ln 2 \\
& + \frac{1}{\beta} \sum_i \left[\left(\frac{\tilde{q}_i + m_i}{2} \right) \ln \left(\frac{\tilde{q}_i + m_i}{2} \right) + \left(\frac{\tilde{q}_i - m_i}{2} \right) \ln \left(\frac{\tilde{q}_i - m_i}{2} \right) \right. \\
& + \left(\frac{(1 - \tilde{q}_i)(1 - \mathbb{T})}{2} \right) \ln \left(\frac{(1 - \tilde{q}_i)(1 - \mathbb{T})}{2} \right) \\
& \left. + \left(\frac{(1 - \tilde{q}_i)(1 + \mathbb{T})}{2} \right) \ln \left(\frac{(1 - \tilde{q}_i)(1 + \mathbb{T})}{2} \right) \right]
\end{aligned} \tag{2}$$

The system is characterized by the following $2N$ coupled TAP-equations.

$$\begin{aligned}
m_i &= \frac{\sinh(\beta H_i)}{\cosh(\beta H_i) + \cosh(\beta \mu) \exp(-\beta X_i)}, \\
\tilde{q}_i &= \frac{\cosh(\beta H_i)}{\cosh(\beta H_i) + \cosh(\beta \mu) \exp(-\beta X_i)},
\end{aligned} \tag{3}$$

where $H_i = h_i^{ext} + \sum_j J_{ij} m_j - \beta m_i \sum_j J_{ij}^2 (\tilde{q}_j - m_j^2)$ and $X_i = \frac{\beta}{2} \sum_j J_{ij}^2 (\tilde{q}_j - m_j^2)$. A third equation for the local filling factors $\nu_i = 1 + (1 - \tilde{q}_i) \tanh(\beta \mu)$ follows from $\nu = -\partial_\mu \mathcal{G}$. In the replicated quantum-field theory the corresponding equation $\nu = 1 + (1 - \tilde{q}) \tanh(\beta \mu)$ turns out to be invariant under an arbitrary number of replica symmetry breaking steps.

2. Convergence and Stability

Inspired by Plefka's work on the non-fermionic system [12] and adopting his replacement $J_{ij} \rightarrow \alpha J_{ij}$ we can rederive the fermionic free energy by a Taylor expansion as follows

$$\begin{aligned}
\mathcal{G}(\alpha) = & -\frac{\alpha}{2} \sum_{ij} J_{ij} m_i m_j - \alpha^2 \frac{\beta}{4} \sum_{ij} J_{ij}^2 (\tilde{q}_i - m_i^2)(\tilde{q}_j - m_j^2) \\
& + \frac{1}{\beta} \sum_i \left[\left(\frac{\tilde{q}_i + m_i}{2} \right) \ln \left(\frac{\tilde{q}_i + m_i}{2} \right) + \left(\frac{\tilde{q}_i - m_i}{2} \right) \ln \left(\frac{\tilde{q}_i - m_i}{2} \right) \right. \\
& + \left(\frac{(1 - \tilde{q}_i)(1 + \mathbb{T})}{2} \right) \ln \left(\frac{(1 - \tilde{q}_i)(1 + \mathbb{T})}{2} \right) \\
& \left. + \left(\frac{(1 - \tilde{q}_i)(1 - \mathbb{T})}{2} \right) \ln \left(\frac{(1 - \tilde{q}_i)(1 - \mathbb{T})}{2} \right) \right] \\
& - \mu \sum_i (1 + (1 - \tilde{q}_i) \mathbb{T}) - \sum_i h_i^{ext} m_i + \frac{N}{\beta} \ln 2 + O(\alpha^3).
\end{aligned} \tag{4}$$

The correct free energy is given by $\mathcal{G}(\alpha = 1)$. The diagrammatic expansion showed already that, provided the series actually converges, the terms of cubic order or higher are suppressed in the thermodynamic limit. We may now determine the radius of

convergence of $\mathcal{G}(\alpha)$, which, by a standard theorem of complex analysis, is equivalent to the radius of convergence of

$$\partial_\alpha \mathcal{G}(\alpha) = -\frac{1}{2} \langle \sum_{ij} J_{ij} \sigma_i \sigma_j \rangle_\alpha = -\frac{1}{2} \sum_{ij} J_{ij} m_i m_j - \frac{1}{2\beta} \sum_{ij} J_{ij} \chi_{ij}(\alpha).$$

There, the susceptibility matrix χ is defined as

$$\chi_{ij}(\alpha) = \beta(\langle \sigma_i \sigma_j \rangle_\alpha - m_i m_j) = \partial_{h_i} \partial_{h_j} \mathcal{F}(\underline{h}, \underline{\chi}).$$

The radius of convergence is given by $\min(|\alpha|)$, where the minimization is done over the values of α with eigenvalues 0 in the inverse susceptibility matrix χ^{-1} . In the non-fermionic case the equation $(\chi^{-1})_{ij} = ([\partial_{\underline{h}} \partial_{\underline{h}} \mathcal{F}(\underline{h})]^{-1})_{ij} = \partial_{m_i} \partial_{m_j} \mathcal{G}(\underline{m})$ signifies that, when taking into account the special properties of the spectra of these random matrices [5], the local stability of a TAP-solution implies the validity of the free energy at this point. In the fermionic model we have to deal with two different matrices to describe either the convergence of the linked cluster expansion $(\chi^{-1})_{ij}$ or the local stability of a given TAP-solution by

$$\begin{pmatrix} \partial_{m_i} \partial_{m_j} \mathcal{G} & \partial_{m_i} \partial_{\tilde{q}_j} \mathcal{G} \\ \partial_{\tilde{q}_i} \partial_{m_j} \mathcal{G} & \partial_{\tilde{q}_i} \partial_{\tilde{q}_j} \mathcal{G} \end{pmatrix} = \begin{pmatrix} \partial_{h_i} \partial_{h_j} \mathcal{F} & \partial_{h_i} \partial_{\chi_j} \mathcal{F} \\ \partial_{\chi_i} \partial_{h_j} \mathcal{F} & \partial_{\chi_i} \partial_{\chi_j} \mathcal{F} \end{pmatrix}^{-1}.$$

A theorem by Pastur [10, 11] used heavily by Plefka [12] and resolvent-calculus can be applied to both cases to determine the limits of the support of the spectra. It is very interesting to note, that at the end of quite lengthy calculations both matrices lead exactly to the same set of conditions generalizing Plefka's convergence and stability conditions by

$$\langle (\tilde{q} - m^2)^2 \rangle \leq T^2 \tag{5}$$

$$\frac{1}{2} \langle \tilde{q}(1 - \tilde{q}) \rangle + 2 \langle m^2 - m^4 \rangle \leq T^2. \tag{6}$$

The known non-fermionic limit is obtained by setting $\tilde{q}_i = 1$. We have thus linked the local stability of TAP-solutions to the finite support of the spectrum of random matrices in the thermodynamic limit. This gives a hint why the numerical search for these solutions is so difficult [4, 16, 17]: for finite N the support of these spectra becomes unbounded, see e.g. [5] for the exponential corrections to the semi-circle-law at finite N . This means, that for every solution the probability of having *negative* eigenvalues in the stability matrix is finite. But already one negative eigenvalue prevents finding this solution via minimization algorithms. Most solutions become thus unstable.

3. Breakdown of the homogeneous paramagnetic solution

The TAP-equations are readily solved numerically in the homogeneous paramagnetic phase, where they reduce to one single equation for $\tilde{q} = \tilde{q}_i$ given for all i by

$$\tilde{q} = \frac{1}{1 + \cosh(\beta\mu) \exp(-\frac{(\beta J)^2}{2} \tilde{q})}. \tag{7}$$

This is exactly the equation found in [6, 9, 14] for \tilde{q} with a replicated quantum-field theory approach.

The second-order transitions between the paramagnetic and the spin glass phase are given by the intersection of the paramagnetic solutions with the stability conditions (equations (5) and (6)). In the next section we find a first order transition on the $T = 0$ axis at $\mu_c \approx 0.8$. We expect a line of first order transitions linking this point with the tricritical point. The dotted line in the phase diagram (figure 1) gives only a schematic behaviour of this line as the exact path is yet unknown.

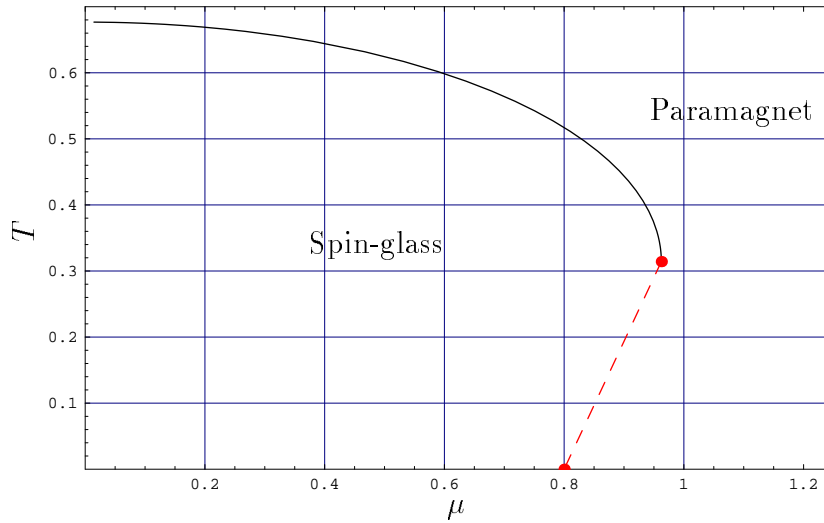


Figure 1. Phase diagram obtained from the fermionic TAP-equations. The dotted line is a linear approximation to the first order transition line connecting the (calculated) tricritical point and the $T = 0$ critical point.

4. TAP-equations at $T = 0$

At $T = 0$ the TAP-equations reduce to

$$m_i = \Omega(h_i), \quad \tilde{q}_i = m_i^2$$

where $h_i = \sum_j J_{ij} m_j$ and $\Omega(x) = \Theta(x - \mu) - \Theta(\mu - x)$ denotes a modified sign function. The energy corresponding to these solutions is simply

$$f_{SG} = - \sum_{(ij)} J_{ij} m_i m_j - \mu \sum_i n_i$$

which has to be compared with the free energy of the paramagnetic solution $f_{PM} = -2\mu$ to find the first order transition. We were able to calculate numerically a huge number of spin glass solutions. We first note the interesting dependence of the

filling factor ν on the chemical potential (see figure 2). Unlike the discontinuous replica-symmetric and finite-step RSB solutions [7, 8] the filling factor varies continuously with μ in the vicinity of $\mu = 0$. The numerical data for the increase of $\nu(\mu)$ near $\mu = 0$ are compatible with power law fits $|\delta\nu| \propto |\mu|^x$, $x > 1$, including exponential behavior.

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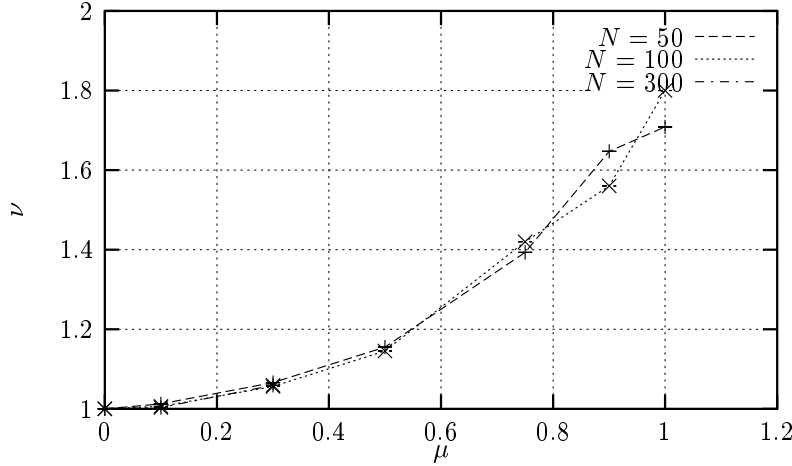


Figure 2. Filling factor $\nu(\mu)$ as a function of the chemical potential for systems of different size.

From the dependence of the energy difference between the spin glass solutions and the paramagnetic solution (figure 3) we can deduce a first order transition at $\mu = \mu_{c1} \approx 0.8$. This critical value of μ can be viewed as a $T = 0$ analogue of the T_{c1} for the thermal first order transitions.

Another very interesting feature shows up in the behaviour of the distribution of the local fields h_i . When applying a chemical potential this probability density function is substantially modified. The “softgap” (see [13]) at $h_i = 0$ splits up into two softgaps at $h_i = -\mu$ and $h_i = \mu$. Within the interval $[-\mu, \mu]$ another peak emerges (see figures 4 and 5).

5. Number of solutions

The number of solutions of the TAP-equations (related to the so-called complexity) can be calculated adopting the procedure of Bray and Moore [1] for finite T or following Roberts [13] for $T = 0$. We were able to obtain in both cases fermionic generalizations of the saddle-point equations, which become extremely complicated due to the additional non-magnetic degrees of freedom. For example in the finite temperature case the

equations for the parameters q , \tilde{q} , η , ϱ , Δ and B read

$$\begin{aligned}
f &= \langle \mathcal{F} \rangle_I, & q &= \langle m^2 \rangle_I, & \tilde{q} &= \langle \kappa \rangle_I \\
0 &= B \left\{ 1 - J^2 \left\langle \frac{(\kappa - (\kappa\lambda)^2)^2}{1 + B(\kappa - (\kappa\lambda)^2)} \right\rangle_I \right\} \\
0 &= \frac{1}{q} \langle \kappa \lambda (\tanh^{-1}(\lambda) - \kappa \lambda \Delta) \rangle_I - \Delta - J^2(\tilde{q} - q) \\
\varrho &= -(\Delta + B) - \frac{J^2}{2} \langle \Theta \sqrt{1 - \lambda^2} \kappa^2 \Xi \rangle_I \\
\eta &= \Delta + B + \frac{1}{2q} \left[1 - \frac{1}{J^2 q} \langle (\tanh^{-1}(\lambda) - \kappa \lambda \Delta)^2 \rangle_I \right] + \frac{J^2}{2} \langle \Theta \sqrt{1 - \lambda^2} \kappa^2 \Xi \rangle_I,
\end{aligned} \tag{8}$$

which can be viewed as an extension of the original equations given by Bray and Moore, but the average $\langle \cdot \rangle_I$ means averaging by use of the following kernel:

$$\begin{aligned}
I &= \int_0^1 d\kappa \int_{-1}^1 d\lambda g(\vec{x}, \kappa, \lambda) \delta(f(\vec{x}, \kappa, \lambda)) \\
&= \int_0^1 d\kappa \int_{-1}^1 d\lambda \frac{\kappa}{\sqrt{2\pi} \sqrt{q} J} \left[\frac{1 + B(\kappa - (\kappa\lambda)^2)}{(\kappa^2 - (\kappa\lambda)^2)} \right] (1 - \kappa)^{u-1} \\
&\quad \times \exp \left(\eta (\kappa\lambda)^2 + \varrho \kappa + \frac{u \kappa \lambda}{2} \tanh^{-1}(\lambda) - \frac{1}{2J^2 q} (\tanh^{-1}(\lambda) - \kappa \lambda \Delta)^2 \right) \\
&\quad \times \delta \left(\ln \left(\frac{(\kappa^2 - (\kappa\lambda)^2) \cosh^2(\mu)}{(1 - \kappa)^2} \right) - J^2(\tilde{q} - q) \right)
\end{aligned}$$

$\lambda = m/\kappa$ is the reduced magnetisation, Ξ an abbreviation for a very lengthy expression. These equations remain currently unsolved even numerically. The equations for $T = 0$ are equally hard to treat.

6. Outlook

The numerical work presented here should now be accompanied by exact analytic RSB calculations for arbitrary μ . In order to reproduce the behavior of $\nu(\mu)$ and of $P(h_i, \mu)$ the generalizations of Robert's saddle-point equations [13] should be solved. It would be desirable to have Parisi's solution (infinite step RSB) for $\mu \neq 0$. The answer to one of the open questions might reveal the exact path of the first order transition line for $T \neq 0$. If this turns out to be impossible, one should find more refined numeric algorithms, which allow to solve the fermionic TAP-equations for $T \neq 0$.

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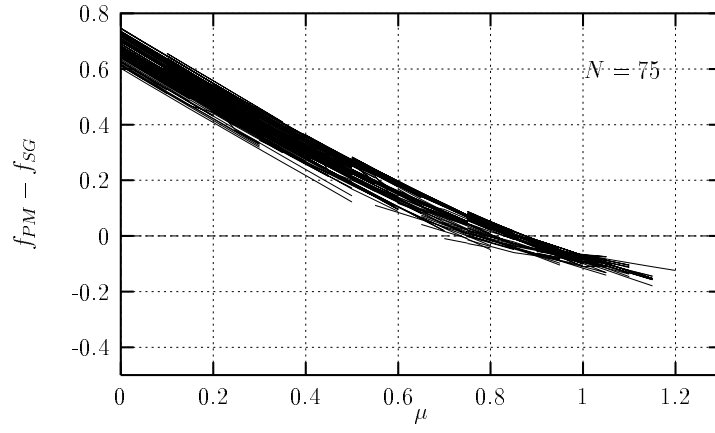
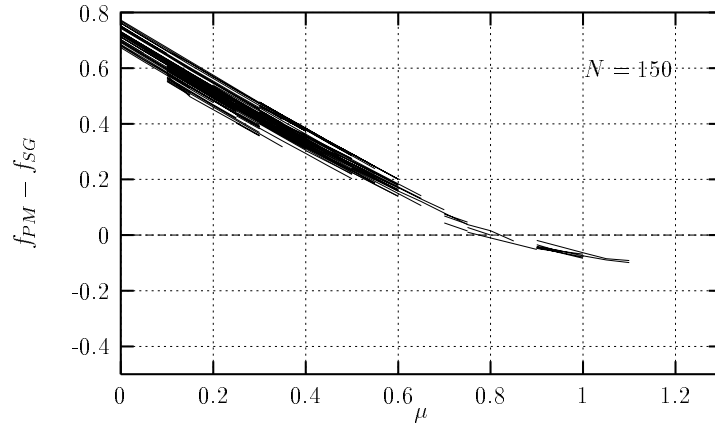
(a) $N = 75$ (b) $N = 150$

Figure 3. Energy gap between spin glass solutions of the zero temperature TAP-equations and the paramagnetic solution for systems of different size.

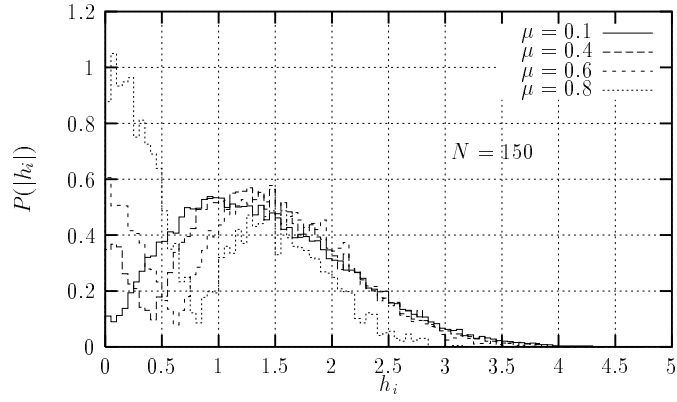


Figure 4. Internal field distribution $P(|h_i|)$ for $N = 150$ and different values of μ . The distribution $P(h_i)$ is symmetric. We used about 10000 points for each histogram.

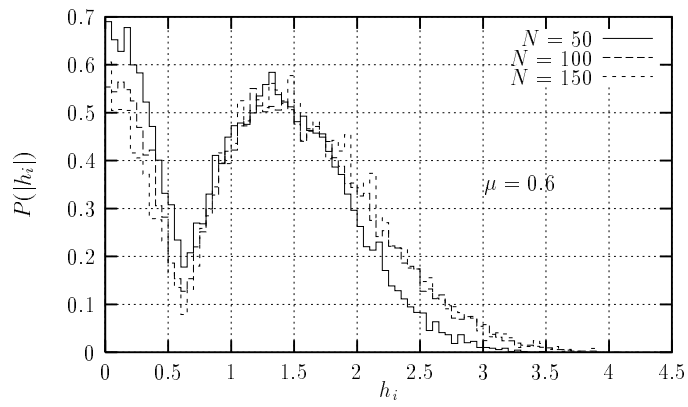


Figure 5. Scaling of $P(h_i)$ at $N = 50$, $N = 100$, and $N = 150$ for $\mu = 0.6$.